D-Glucitol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.85e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 4.02e-01

Confidence level: 7.85e-01

Nearest Neighbors from the Training Set

Image not found
2-(2-Butoxyethoxy)ethanol
Measured: 7.44e-11
Predicted: 5.15e-11

Image not found
2-(2-Ethoxyethoxy)ethanol
Measured: 5.72e-11
Predicted: 3.59e-11

Image not found
1-Butoxy-2-propanol
Measured: 3.76e-11
Predicted: 3.73e-11

Image not found
Propane, 1,1,3-trimethoxy-
Measured: 1.92e-11
Predicted: 2.33e-11

Image not found
3-Methoxybutan-1-ol
Measured: 2.36e-11
Predicted: 2.52e-11